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Calculated melting curves for phases of iron

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ABSTRACT

We present a method by which the melting curves and corresponding densities along the liquidus of iron phases are calculated at high pressure. The melting curve of the ε(hcp) iron phase is calculated from $P = 0$ to $P = 330$ GPa. The melting curve of the γ_i(fcc) iron phase is calculated from $P = 0$ to $P = 100$ GPa. The point where these curves cross, near $P = 50$ GPa, is the location of the upper triple point on the melting curve.

Our method combines the Lindemann melting equation with the Vinet isothermal equation of state. These equations are coupled by means of the Grüneisen parameter, γ, which is given by K_T' (the pressure derivative of the isothermal bulk modulus, K_T) of the equation of state. By this thermodynamic formalism, we find values of volume, V; temperature, T; and the Grüneisen parameter, γ, along the melting curve. This calculation requires the following thermal parameters: thermal expansivity, α_V, at high T; $(\partial K_T/\partial T)_P$ at high T; the melting temperature, T_m, at $P = 0$; $q = (\partial \ln \gamma/\partial \ln \rho)_T$ at high T; and γ. The method also requires zero-pressure equation-of-state parameters: density, ρ, at $T = 300$ K; K_T at $T = 300$ K; and $(\partial K_T/\partial P)_T$ at $T = 300$ K. Our results do not confirm or deny the existence of the recently proposed β phase. We demonstrate that with our existing knowledge the physical parameters of the β and ε phases may be so close to each other that these two phases need not be considered separately in discussing the physics of iron at core P,T conditions. We find that one set of reasonable thermoelastic parameters of the ε phase reproduces the melting temperature and density at pressures of 50 and 240 GPa. Further, these parameters give agreement with previous estimates of the melting temperature and density at 330 GPa.